Experimental boundary conditions for frequency domain PDW spectroscopy – a Monte Carlo study

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To characterize the optical properties of strongly light scattering materials, like polymer dispersions, paint, food, or cosmetics, different experimental techniques can be used, e.g. spatially or time-resolved reflectance or transmission measurements or Photon Density Wave (PDW) spectroscopy in the frequency domain. Here, the radiative transfer equation is often applied in data analysis to determine the absorption (μ_a) and reduced scattering coefficient (μ_s') from the measured signals. Additionally, the diffusion approximation (DA) with appropriate boundary conditions is widely used due to the simplicity of the solution. However, the DA restricts the data analysis to samples with an absorption coefficient that is small compared to the reduced scattering coefficient ($\mu_a<<\mu_s$') and too small modulation frequencies. Especially because of the latter condition the solution of the radiative transfer equation in the P1-approximation for an infinite medium has been used for PDW spectroscopy quite extensively and has been applied successfully to determine the optical properties and subsequently particle sizes with high precision and accuracy [1–2]. However, the boundary conditions used to derive the P1-approximation include an infinite sample volume and an isotropic point-like light source and detector which can only be achieved to a certain extent experimentally.

To study the influence of the above mentioned conditions and further experimental influences on the results of PDW spectroscopy Monte Carlo (MC) simulations are carried out to simulate the light expansion in the sample. The simulated amplitude and phase of the PDW are compared directly to the P1-approximation to identify major influences. Additionally, the simulated MC data are analyzed via the P1-model and the influence of different experimental parameters including sample volume, range of relative and absolute fiber positions as well as modulation frequencies and fiber parameters on the resulting optical coefficients is evaluated with respect to the accuracy of the latter. In case of the above mentioned materials, the infinite medium is well approached by sample volumes typically ranging from 50 mL – 1 L depending on the optical properties and a not too small absorption coefficient (to reduce loss of light at the sample boundaries). The isotropy and point-like dimension of the light source and the detector can be approximated by using optical fibers with high numerical aperture and small fiber core to couple light into or out of the sample. Depending on the optical parameters and fiber properties, data analysis should be carried out excluding e.g. too small distances between emission and detection fiber to obtain results with high accuracy and precision.

References

[1] Bressel, L., Hass, R., and Reich, O., 2013: Particle sizing in highly turbid dispersions by Photon Density Wave spectroscopy. *JQSRT* **126**, 122–129.
[2] Hass, R., Münzberg, M., Bressel, L., and Reich, O., 2013: Industrial applications of Photon Density Wave spectroscopy for in-line particle sizing. *Appl. Opt.* **52**, 1423–1431.

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